April 2011

MPA MaterialsMatter

INSIDE

Ross McDonald

Aiming for the heart of the matter

By Francisco Ojeda
ADEPS Communications

Since he was a toddler, Ross McDonald has been fascinated by how things work. When he was 3 years old, he dismantled his parent's vacuum, piece-by-piece, down to the motor. Luckily, instead of punishing him, his parents praised his ingenuity.

"I've always wanted to find out how things worked," McDonald said. "That's why I enjoy physics so much. It's about seeking an understanding, with less emphasis on remembering facts than other areas of science. It's about trying to understand, often quite obscure, phenomena."

McDonald is a condensed matter physicist at Los Alamos National Laboratory's National High Magnetic Field Laboratory Pulsed Field Facility. There, he explores the physical properties of matter in an attempt to understand their behavior using well-established physical laws, such as electromagnetism, quantum mechanics, and statistical mechanics.

"I always try to answer the 'why' question—why does something happen or not happen," said McDonald of Condensed Matter and Magnet Science (MPA-CMMS). "I am naturally curious. I enjoy being in the lab and trying to find out things no one else has discovered yet."

At the magnet lab, McDonald has developed new instrumentation for conducting gigahertz-frequency complex-conductivity experiments in millisecond duration pulsed magnetic fields, which he is currently extending to higher intensity and shorter duration magnetic fields. His expertise includes a wide variety of experimental techniques to measure correlated electron systems in high magnetic fields.

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From Toni's Desk

I am going to use this column to provide several updates on various issues concerning LANL and MPA Division.

First, I have some good news on space. The Laboratory is providing institutional funding to construct new lab space for MPA-MC in the unfinished space on the second floor of the Materials Science Laboratory (the MSL infill). The plan is for construction of this space to be completed by July 2012 and the non-rad MPA-MC activities at TA-48 to move to the MSL by the end on FY12. MPA-11 has also received support to refurbish the former plating shop space at SM-40. MPA-11's fuel cell labs at TA-46 will then move into this space.

The call for LDRD-DR proposals was recently announced. MPA was quite successful in this call with full proposals requested for the following white papers from MPA PIs:

- Plutonium-242: A National Resource for the Fundamental Understanding of 5f Electrons (PI: Eric Bauer, MPA-CMMS)
- Moment Formation in 3d-Electron Metals (PI: Joe Thompson, MPA-CMMS)
- Genetically Encoded Materials: Libraries of Stimuli-responsive Polymers (PI: Jennifer Martinez, MPA-CINT)
- Acoustic Engineering of New Materials with Designed Properties (PI: Dipen Sinha, MPA-11)
- Energy Storage (PI: Tony Burrell, MPA-MC)

In addition, MPA investigators play key roles in invited proposals led by MST, T, AOT, and B Divisions. Full proposals are due May 5. I also know that many excellent pre-proposals were not included in the call for proposals. David Watkins and I will work with those proposal teams to find alternate funding and/or strengthen those proposals for next year's LDRD-DR competition.

Updates on space, LDRD-DR proposals, the search for a new Laboratory Director, and the budget uncertainty.

I know that there is anxiety about the search for the new Laboratory Director. I am a member of the Screening Task Force for the new Director that will screen a list of more than a hundred candidates against a set of criteria and then present a list of 10-15 names to the Search Committee by mid-April.
The Search Committee will then evaluate those candidates through a series of interviews and discussions and present a short list of candidates to the president of the University of California and to the chair and vice-chair of the board of governors. It seems to me that this process is proceeding smoothly and expeditiously, so that there may well be a new Director chosen, if not on-board, by the time Mike steps down on June 1.

In closing, I appreciate that the budget uncertainty is a distraction for all of us and makes planning our future activities very difficult. I would like to emphasize the Director's message at his recent all-hands meeting, "It's really important that we stay focused and that we execute; that's our best defense against the current budget uncertainty."
I know that the MPA can and will continue to produce forefront S&T, even in these trying times.

MPA Division Leader Toni Taylor

MPA MaterialsMatter

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To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or kkippen@lanl.gov.

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To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml

McDonald . . . Recently he helped a group of external collaborators develop a novel approach to isolate signs of electrical current flowing along the surface of a topological insulator, a material with intriguing electrical properties, and which could lead to new fundamental physics discoveries.

"It's exciting because we are exploring something new, and we were able to use the high magnetic fields at the magnet lab to solve the problem," McDonald said.

The researchers are currently concerned with exploring the fundamental properties of the material, but are also interested in how this research might enable future applications of topological insulators.

"Ross went the extra mile to help make the experiment successful," said MPA-CMMS Deputy Group Leader and Pulsed Field Facility Director Chuck Mielke.

Attracted to new ideas, new experiments

McDonald, who is from London, earned his PhD in condensed matter physics from the University of Oxford in 2001. While at the university, he took a short educational trip to Los Alamos, where he learned of a postdoctoral research position at the magnet lab. After graduation, McDonald began working at the Laboratory with his mentor Neil Harrison (MPA-CMMS).

"He is a highly gifted experimentalist," Harrison said of McDonald. "He can do a variety of things in the lab and he develops concepts quickly." According to Harrison, McDonald's broad knowledge of condensed matter physics spreads into piezoelectric cantilever magnetometry, optical conductivity, electron-paramagnetic resonance and high-pressures and magnetic fields.

McDonald said his favorite aspect of working at the magnet lab is the user program, in which he spends about 25 percent of his time supporting users. Through a National Science Foundation grant to aid visiting magnet lab scientists, McDonald collaborates with international scientists and offers his scientific expertise to ensure successful experiments. He assists users with all aspects of the experiment, from set up to development of samples to scientific advice.

McDonald said he enjoys the user support program because it provides opportunities to be exposed to new ideas and topics, to work with different scientists, and to start new collaborations. "It's a very refreshing environment because things are changing all the time," he said. "You are doing new things all the time and learning what other scientists are doing with their research."

McDonald happens to be good at it, too.

"He is one of the best user support scientists the magnet lab has," Mielke said. "He goes above and beyond to help users. They explicitly ask to work with Ross."

That's because he seeks to understand.

McDonald's favorite experiment

What: Observing Dirac fermions on the surface of a topological insulator
When: First conclusive observations of the two-dimensional surface-state, fall 2009.
Where: National High Magnetic Field Laboratory, Pulsed Field Facility at Los Alamos National Laboratory.
Why: Despite the wide range of physical phenomena I've observed, I find it hard to top seeing magnetic quantum oscillations. This is partially because the data sets are so aesthetic, and partially because of the challenge of resolving such small oscillatory changes in the magnetization or conductivity. But mainly the reason is because of the richness of the information conveyed about how the electrons in the material behave–the dimensionality, the influence of interactions and the scattering rate. The topological insulator experiment is a particularly memorable example, both because of the technical challenges, and the impact of the result.
How: By measuring in the world's highest available magnetic fields, we were the first to observe the conductivity signature of the metallic state that was predicted to exist on the surface of a new class of materials.
The a-ha moment: Came when we rotated the sample to reveal that the oscillations only depended upon the component of magnetic field perpendicular to the surface, thus distinguishing them from three-dimensional bulk effects.

Tuning the resonance in high-temperature superconducting terahertz metamaterials

Metamaterials consisting of metallic elements enable a structurally scalable electrical and/or magnetic resonant response, from which exotic electromagnetic phenomena absent in natural materials have been observed. Metals provide high conductivity necessary to produce strong electrical and magnetic metamaterial response. However, they play a negligible role in active and dynamical metamaterial resonance switching and/or frequency tuning. These processes are typically accomplished through the application of external stimuli when other natural materials (e.g., semiconductors)

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Tuning... or devices are integrated into metamaterials. Modification of the metamaterial embedded environment contributes to such previously observed functionalities and their unprecedented performance. At low temperatures, superconducting materials possess better conductivity than metals at frequencies up to terahertz. Therefore, superconducting metamaterials are expected to have lower loss than metal metamaterials.

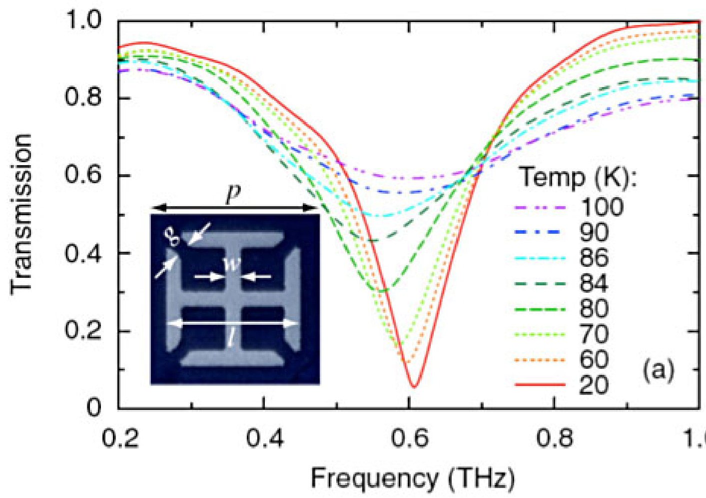
LANL researchers have fabricated and characterized electric split-ring resonator-based metamaterials from high temperature superconducting YBCO films. Their work reveals, for the first time, the unique phenomena produced by combining these materials and offers the tantalizing prospect of the development of novel, multifunctional metamaterials realized through use of this hybrid material.

The scientists discovered resonance properties in terahertz metamaterials consisting of a split-ring resonator array made from high-temperature superconducting films. By varying the temperature, they observed efficient metamaterial resonance switching and frequency tuning. The results are well reproduced by numerical simulations of metamaterial resonance using the experimentally measured complex conductivity of the superconducting film. The researchers developed a theoretical model that explains the tuning features, which takes into account the resistive resonance damping and additional split-ring inductance contributed from both the real and imaginary parts of the temperature-dependent complex conductivity. The theoretical model predicts more efficient resonance tuning in metamaterials that consist of a thinner superconducting split-ring resonator array. The scientists verified the prediction experimentally. The findings pave an avenue towards novel functional terahertz metamaterials by simultaneously taking advantage of the unique properties in metamaterials and complex oxide materials.

Researchers include Hou-Tong Chen, Ranjan Singh, John O'Hara, Abul Azad, and Q. X. Jia (Center for Integrated Nanotechnologies, MPA-CINT); Hao Yang (formerly MPA-CINT, currently Soochow University, China); Stuart Trugman (MPA-CINT and Physics of Condensed Matter and Complex Systems, T-4); and Antoinette Taylor (Materials Physics and Applications, MPA-DO).

Reference: "Tuning the Resonance in High-Temperature Superconducting Terahertz Metamaterials," *Physical Review Letters* **105**, 247402 (2010). The Laboratory Directed Research and Development (LDRD) Program funded the research, which supports the Lab's Materials for the Future capability pillar.

Technical contact: Hou-Tong Chen



THz transmission amplitude spectra of the 180-nm thick YBCO metamaterial at various temperatures.

Paper among top 25 from Institute of Physics's celebration of 100 years of superconductivity

The discovery, by Los Alamos researchers and collaborators, of pressure-induced superconductivity in $CaFe_2As_2$, has been selected for its relevance and impact as one of only 25 papers from among hundreds in five Institute of Physics (IOP) journals as part of its centenary celebration of superconductivity. The top 25 includes a selection of articles on the newly discovered iron-based superconductors and a selection of articles by Nobel Prize Laureates. The selected articles have been chosen from five journals published by IOP Publishing: *Superconductor Science and Technology, Journal of Physics: Condensed Matter, New Journal of Physics, EPL,* and *Physica Scripta.*

The article, by Tuson Park (Condensed Matter and Magnet Science, MPA-CMMS and Sungkyunkwan University, Korea), and collaborators Eunsung Park (Sungkyunkwan University), former MPA-CMMS postdoctoral researchers Hanoh Lee (Stanford University) and Tomasz Klimczuk (Institute for Transuranium Elements), and Eric Bauer, Filip Ronning, and Joe D. Thompson (MPA-CMMS); appears in a commemorative brochure available at a variety of conferences in 2011 and on the IOP Web site (iopscience.iop.org/page/centenary).

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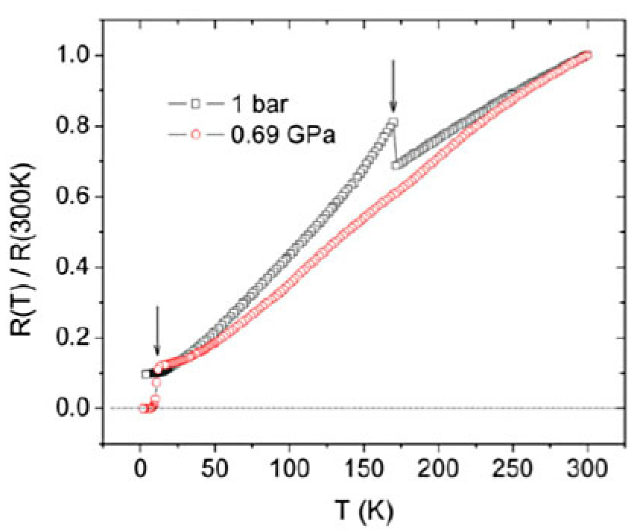
Paper... In their paper, the scientists report pressure-induced super-conductivity in a single crystal of $CaFe_2As_2$. This is the first of the Fe-As-based $ThCr_2Si_2$ structure-type materials to exhibit such phenomena (see figure). Its superconducting transition temperature at 0.69 GPa is relatively high, approaching 25–50% of the highest Tcs reported for hole doped AFe_2As_2 materials, where A is calcium, strontium, or barium. These observations reveal that pressure offers a new route to superconductivity in these and possibly the related ZrCuSiAs-structure materials without the need to introduce extrinsic chemical disorder.

Since its 2008 publication, the paper has been cited more than 90 times, reflecting its importance to the understanding of the superconducting mechanism of $CaFe_2As_2$ and other Fe-based high-T_c superconductors. Reference: "Pressure-induced Superconductivity in $CaFe_2As_2$," *the Journal of Physics: Condensed Matter* **20**, 322204 (2008).

The Los Alamos research was performed under the auspices of the DOE Office of Science, Division of Materials Science and Engineering and supported in part by the Los Alamos Laboratory Directed Research and Development (LDRD) program. The work supports the Lab's Energy Security mission area and the Materials of the Future capability pillar.

Technical contact: Tuson Park or Mike Hundley



Temperature dependence of the normalized resistance of $CaFe_2As_2$. Resistance divided by its room-temperature value is plotted against temperature for 1 bar (squares) and 0.69 GPa (circles). For reference, the room-temperature resistivity is approximately 0.22 mΩ cm at atmospheric pressure. Arrows indicate magnetic and superconducting transitions for 1 bar and 0.69 GPa, respectively.

Katherine Lovejoy appointed Reines Postdoctoral Fellow

Postdoctoral researcher Katherine Lovejoy (Materials Chemistry, MPA-MC) has been awarded the 2011 Frederick Reines Postdoctoral Fellowship in Experimental Sciences. Lovejoy joined the Laboratory in December 2009 as an Intelligence Community Postdoctoral Fellow. She worked on the design and synthesis of non-aqueous liquid materials for use in forensic applications by the FBI.

The project involved development of a strategy for advanced analysis of dyes on wool fibers found at improvised explosive device (IED) explosion sites. Her research has resulted in a primary-author article in Analytical Chemistry (in press), and a U.S. patent application has been filed. Her LANL mentors are Rico Del Sesto (MPA-MC) and Andy Koppisch (Bioenergy and Environmental Science, B-8).

As a doctoral bioinorganic chemistry student at the Massachusetts Institute of Technology working with Steve Lippard, Lovejoy led external collaborations to advance platinum anticancer drug candidates through pre-clinical trials, including performing in vitro and in vivo studies at several international university and hospital laboratories. Her research resulted in a patent application and several publications, including an article in the *Proceedings of the National Academy of Sciences* that described a platinum antitumor agent. Lovejoy received an International Precious Metals Institute Student Award for her research in the field of precious metals. She also studied at Germany's Max Planck Institute for Polymer Chemistry on a Fulbright Grant, where she helped discover a robust model membrane system that led to a DARPA (Defense Advanced Research Projects Agency) grant.

The Reines is one of three Laboratory Distinguished Postdoctoral Fellowships, the recipients of which must display extraordinary ability in scientific research and show clear and definite promise of becoming outstanding leaders in the research they pursue. This Fellowship, which supports experimental science, is named after the former LANL researcher who won the 1995 Nobel Prize in Physics.

Michael Nastasi named 2011 Materials Research Society Fellow

Michael Nastasi (MPA-CINT) has been selected as a 2011 Materials Research Society (MRS) Fellow. The Fellows are recognized as outstanding MRS members whose sustained and distinguished contributions to the advancement of materials research are internationally recognized. Each year, no more than 0.2 percent of the current membership of the Society is elected to the status of Fellow. Nastasi's award citation read, "For seminal contributions to the field of ion-solid interactions and radiation effects, including synthesis of novel materials using energetic ions, with applications to energy, manufacturing, nanotechnology, and advanced microelectronics." He will be formally recognized during the 2011 MRS Spring Meeting in San Francisco.

Nastasi has a PhD in materials science and engineering from Cornell University. He is the director of the Center for Materials at Irradiation and Mechanical Extremes (CMIME). Previously, Nastasi was the nanoelectronics and mechanics thrust leader at the Center for Integrated Nanotechnologies and the team leader of the nanoscience and ion-solid interaction team in Structure/Property Relations (MST-8). His research interests include irradiation effects in nanostructured materials, irradiation induced phase transformations, ion enhanced and plasma synthesis of materials, mechanical properties of metastable materials and nanoscale structures, and materials analysis using ion beam techniques. He is a Fellow of America Physical Society and Los Alamos National Laboratory. Founded in 1973, the MRS consists of more than 15,100 members from the United States – as well as nearly 70 other countries. The Society is different from that of single discipline professional societies because it encourages communication and technical information exchange across the various fields of science affecting materials.

Technical contact: Michael Nastasi

Celebrating service

Congratulations to Anatoly Efimov, MPA-CINT, who celebrated his 10-year service anniversary this month.

Shadi Dayeh receives Postdoctoral Distinguished Performance Award

Shadi Dayeh (MPA-CINT) is the recipient of a 2010 Postdoctoral Distinguished Performance Award in recognition of his outstanding performance that has made a significant contribution to the Laboratory.

Dayeh, a Distinguished J. Robert Oppenheimer Postdoctoral Fellow, was recognized for his outstanding contributions to the research and development community through his scientific accomplishments and creative ideas. His mentor, Tom Picraux (MPA-CINT) nominated him.

Dayeh used the vapor-liquid-solid method to develop the most complete treatment of size-dependent growth of germanium nanowires. This comprehensive study potentially settles the controversial area of the size-dependent growth rate of nanowires. Dayeh has also worked on heterostructured nanowire growth and devices, and most notably uncovered issues surrounding the growth of core/shell germanium/silicon (Ge/Si) nanowires for field effect transistors that showed record on-current performance and utilized bandgap engineering in axial Ge/Si heterostructured nanowires for high on/off current switches. In addition, he has proposed a new research approach for neural probes that could open a new area of neuronal studies. Dayeh is the principal investigator of a Laboratory Directed Research and Development–Exploratory Research proposal on "High Density Neuronal Recording using Nanowire Capacitor Sensors."

He came to LANL as a Director's Postdoctoral Fellow after earning his PhD in electrical and computer engineering/electronic materials and devices from the University of California, San Diego in 2008. Dayeh has served as vice president and president of the Los Alamos Postdoc Association, and he initiated an annual Los Alamos Postdoc Research Day.

From David's Desk

Much of the Division is aware that MPA-CINT is the home for the Center for Integrated Nanotechnologies. Some people may be less aware of our role as a DOE Office of Science National User Facility. I'd like to take this opportunity to bring CINT, the User Facility, to everyone's attention, and to encourage you to engage us to support you in your research efforts.

CINT is one of five DOE Basic Energy Sciences-sponsored Nanoscale Science Research Centers (NSRCs) across the country. All five centers are operated as national user facilities to support international research in nanotechnology. CINT has several important characteristics that differentiate us from the other four centers. We are the only center that is jointly operated as a partnership between two national laboratories, Los Alamos and Sandia National Laboratories. This allows us to capitalize on the traditional strengths and talents of both labs through our Core facility at SNL and our Gateway facility at LANL. We are also the only center that resides within a National Nuclear Security Administration host lab. This is an important advantage because it exposes our users to important mission-related research areas and gives our CINT scientists the opportunity to make scientific contributions in support of these missions. One additional differentiating characteristic at CINT is our focus on nanoscience integration. Working with our users, we seek to combine diverse classes of nanomaterials across length scales from nano- to microscale to design and achieve new properties and new functionality. Clearly if we are to realize the ultimate benefit of nanotechnology, integration to achieve device-scale functionality is key.

'Working with our users, we seek to combine diverse classes of nanomaterials across length scales from nano- to microscale to design and achieve new properties and new functionality.'

The NSRCs are an entirely new breed of user facility that emphasizes strong collaboration between our users and our staff. This can be contrasted with the more traditional DOE user facilities such as the synchrotron light sources that provide experimental access to end-stations for users to perform fairly well defined measurements. Our CINT scientists at LANL and SNL (currently ~ 40 in number) each receive ~ 0.5 FTE per year to support our user community. For this level of operational support, each CINT scientist typically provides collaborative support to ~ 5 - 8 user projects ongoing at any time. This research support runs the gamut from design and planning of experiments, syntheses of samples, collection and analysis of data, and in most cases to preparation of joint publications. While users can and do engage us only for access to specific instrumental capabilities foregoing the collaborative interactions with our staff, this is more the exception than the norm. Notably, each CINT scientist derives the other half of his/her support through program development in LDRD, DOE, and other sources. These other programs are synergistic with our CINT internal science and include some familiar high-profile examples, including the LANL-led Energy Frontier Research Centers.

Our scientific focus is organized around four thrusts; 1) nanophotonics and optical nanomaterials, 2) nanoscale electronics and mechanics, 3) soft, biological, and composite nanomaterials, and 4) theory and simulation of nanoscale phenomena. Each thrust maintains a core set of capabilities and competencies for our users defined by the scientific strengths of the thrust members. Of equal importance, the thrusts also work as a team to pioneer new areas of nanoscale science within and at the interface between the thrusts and to develop entirely new tools to meet specific challenges associated with nanomaterial characterization and performance. We believe this pioneering work keeps us optimally positioned to meet new user demands and anticipate the next great advance in nanotechnology. Recent examples include our new signature initiatives called "integration focus activities" in the areas of (a) nanowires for new energy concepts, (b) membrane-based nanocomposites, and (c) metamaterials and plasmonics. These IFAs are explicit cross-thrust efforts that leverage thrust and Center strengths to address broader nanoscience integration challenges and provide a mechanism to link our users into a larger research community.

We have added many exciting new instrumental capabilities and scientific focus areas to our repertoire in the past 18 months, including a new concerted effort in carbon nanomaterials. I encourage everyone to visit our Web site, cint.lanl.gov, to explore our many capabilities and instruments, and to consider submitting a user proposal to access our Center and work with our staff. Approximately one-third of our user community comes from within the technical staff at Sandia or Los Alamos. We are grateful for this "local" business and look forward to collaborating with many of you in the near future.

David Morris, Director,
Center for Integrated Nanotechnologies

Teaming up to provide solutions

Want to help your co-workers find answers to safety and security issues that leave them frustrated and unable to get their work done efficiently? Consider volunteering to serve on your group's Solutions Team.

Begun this year, the three-member teams, composed of an R&D staff member, one Worker Safety and Security Team (WSST) member and a technician or research technologist, perform peer-to-peer walkarounds of work areas with the intent of finding and fixing vulnerabilities on the spot.

"You're doing your coworkers a favor by pointing out potentially hazardous situations, helping them get the resources they need, and documenting trends you're not even aware of," said Eve Bauer of the Materials Chemistry (MPA-MC) Solutions Team and chair of the Materials Physics and Applications WSST.

Housekeeping, waste reduction, and electrical issues are some of the more common challenges taken up by the teams, Bauer said. "In one of our walkarounds we noticed an exposed wire in an 110 outlet and we were able to get that fixed right away. It didn't get lost in the system," she said. The electrical safety officer was called in to check the space and offered safe alternatives to the "daisy chaining" (plugging into each other) extension cords.
Teams are required to document their findings and present an informational summary at the end of their term to the ADEPS Council that captures the overall evaluation of the safety culture and identifies problem areas and deficiencies.

"Solutions Teams look out for our colleagues by helping them get the resources they need to do their work in a safe and secure manner."

Associate Director Experimental Sciences
Susan J. Seestrom

Team members serve for about three months and participation generally requires about an hour and half of a person's time. "You can get as involved as you want," Bauer said.

To volunteer for a Solutions Team, to schedule a walkaround, or for more information, contact one of your group's WSST members.

Your WSST members

MPA: Eve Bauer, Mike Torrez, Paul Mombourquette, John Rowley, Lisa Phipps
LANSCE: Jean Trujillo, Nathan Okamoto, Hank Alvestad, Phil Chacon, Fermin Gonzales, Dominic Tafoya, Victor Vigil, Vince Melito, Thomas Spickermann, William Roybal, John Lyles, Howard Nekimken, Eric Larson, John Ullmann, Leo Bitteker, Dan Seely, Carl Morgan, John Graham, Kristy Ortega , John Erickson (champion), Kurt Schoenberg (champion)
MST: Erik Luther, Dave Alexander, Diana Honell, Stephanie Tornga, Thomas Sisneros, Andy Nelson, Sue Duncan
Physics: Jeff Bacon, June Garcia, Larry Rodriguez, Robert Aragonez, George Sandoval, Todd Womack

Meeting planning services available

Got a conference that needs organizing, an event to be planned?

Rose Romero, the ADEPS meeting coordinator, can help.

With 15 years of Los Alamos conference planning experience, Romero has assisted staff members in planning conferences both large and small, from locally held meetings with a dozen participants to international conferences for hundreds of attendees. Knowledgeable in the Laboratory's conference management policies and associated allowable conference costs, she can help in overseeing the details that ensure a smooth, successful event.

Romero can assist with developing and overseeing allocated workshop budgets, obtaining the necessary cost codes for workshop funding, negotiating and overseeing contracted food services, and in planning and executing workshop and conference web sites. Her experience includes arranging for transportation, conference facilities, and accommodation and preparing pre-conference materials such as invitation letters, badges, folders, and participant lists. During the workshop, she can manage the registration desk, help in setting up meeting rooms, and in compiling agenda, abstracts, and related materials into post-conference documents.

"I love the variety and working on things from start to finish," Romero said. "Meeting planning is like putting together a puzzle. Every piece must fit the puzzle for the puzzle to be successfully complete."

Romero can be reached by calling 665-7657or e-mailing rbromero@lanl.gov.